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**MOLECULAR STRUCTURE OF BIS (2,2-DINITROPROPYL)-
NITRAMINE (BDNPN): POSSIBLE RDX REPLACEMENT**

A. J. Bracuti

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13. ABSTRACT (Maximum 200 words) An x-ray diffraction single-crystal structure determination of Bis(2, 2-dinitropropyl)-nitramine (BDNPN) was carried out. Bis(2, 2- dinitropropyl)-nitramine has the molecular formula C ₆ H ₁₀ N ₆ O ₁₀ and a density of 1.78 g/cc. It crystallizes with two formula weights in the C-centered monoclinic space group C2 (no. 5) with unit cell parameters a = 10.726(4) Å, b = 5.992(3) Å, c = 10.400(4) Å, and β = 110.01(3) deg. The positions of the atoms were determined with both direct methods and difference Fourier techniques. The structure was refined to a final R value of 0.036. The crystal structure consists of BDNPN molecules oriented along the c axis at 000 and 220. The crystal is held together by van der Waals forces between each molecule and its six nearest-neighbors. The molecule is composed of two gem-dinitropropyl groups bonded to a central nitramine group. A comparison of the thermochemical data of BDNPN, cyclotrimethylenetrinitramine (RDX), and 1, 3, 3-trinitroazetidine (TNAZ) reveals that BDNPN has the highest Impetus and lowest flame temperature within this group of molecules.				
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INTRODUCTION

For many years cyclotrimethylenetrinitramine (RDX) has been the oxidizer of choice in high energy/density propellant formulations because of its high density (1.8 g/cc) and energy content (Impetus 1408 J/g). Cyclotrimethylenetrinitramine is a heterocyclic molecule which contains three nitramine groups which alternate in the ring with three methylene groups.

Despite the success of RDX in high energy/density propellant formulations, recent Army goals to reduce or minimize propellant vulnerability have renewed interest in alternate oxidizers because of some problems RDX has with respect to sensitivity to extraneous stimuli, such as shaped-charge impact and shock.

In an effort to improve propellant sensitivity to extraneous stimuli, other high energy/density molecules are being sought as possible candidates for use in both solid and gel slurry/propellant formulations.

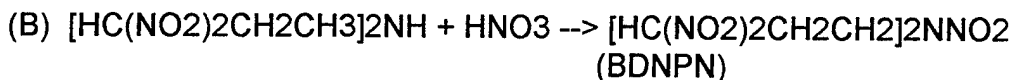
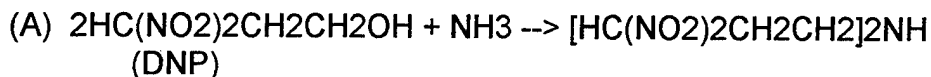
Like the proverbial chain, a molecule is only as stable as its weakest intramolecular bond. Propellant oxidizers usually are molecules which contain multiple oxygen-rich substituents such as nitrate ester groups (O-NO₂), nitramine groups (N-NO₂), or nitro groups (C-NO₂). With these molecules, decomposition most likely starts with scission of the bonds between the substituents and the parent molecule. These bonds would then be the weak links in the molecule. The critical bonds for the nitrate ester group, the nitramine group, and the nitro group substituents are O-N, N-N, and C-N, respectively. The order of relative bond energies for these bonds is C-N > N-N > O-N (ref 1). The greater the bond energy, the more stable the bond.

If one uses bond energies as a crude rule of thumb for designing or selecting molecules to improve propellant stability, then molecules containing multiple nitro groups should be considered potentially more stable than those with multiple nitramine or nitrate-ester groups. It is also believed that the substitution of two nitro groups on the same carbon atom (geminal conformation, or gem-dinitro) is a more stable configuration than single substitution of two nitro groups on different carbon atoms.

One molecule which has been considered as a possible replacement for RDX is 1,3,3-trinitroazetidine (TNAZ). In contrast to RDX with its three nitramine groups, this four-membered heterocyclic molecule also has three NO₂ units, but only one of which is a nitramine, while the others are bonded in the gem-dinitro configuration.

Another molecule which also may have potential for replacing RDX is bis(2,2-dinitropropyl)-nitramine (BDNPN). This molecule, like TNAZ, has only one nitramine group, but unlike TNAZ, it has two gem-dinitro groups and is not heterocyclic.

A two-step reaction scheme to synthesize BDNP has been devised (ref 2), which uses commercially available 2,2-dinitropropanol as the starting material. Initially in this scheme, as shown in step A, 2,2-dinitropropanol is reacted with ammonia to form bis(2,2-dinitropropyl)-amine which then, as indicated in step B, is reacted with nitric acid to form BDNP.



In order to determine unequivocally if this reaction scheme actually produces BDNP, a single-crystal x-ray diffraction investigation was initiated to determine the crystal and molecular structure of the reaction product.

EXPERIMENTAL

X-Ray Diffraction Data Collection

Colorless plate-like single crystals of the reaction product were obtained by recrystallization from tetrahydrofuran. A selected crystal with dimensions of about 0.1 by 0.2 by 0.4mm was mounted on a glass fiber with its long axis approximately parallel to the goniometer phi axis. The preliminary examination and subsequent data collection were performed with Cu K α x-rays ($\lambda = 1.54178 \text{ \AA}$) on an Enraf-Nonius computer controlled kappa-axis CAD4 diffractometer equipped with a graphite incident beam monochromator.

All x-ray diffraction measurements were made at $23 \pm 1^\circ\text{C}$. The lattice constants (table 1) and orientation matrix from least squares refinement using setting angles 23 reflections in the range $9^\circ < \theta < 24^\circ$.

The intensity data were collected to a maximum 2θ value of 150.0 using the $\omega - \theta$ scan technique with a scan rate varying from 2 to $20^\circ/\text{min}$ (in ω) and an $\omega - \theta$ scan speed ratio of 1.5 to 1.

As a check on crystal and electronic stability, three representative reflections were measured every 41 min. The intensities of these standard reflections remain constant within experimental error throughout the course of data collection.

Data Reduction

A total of 1,345 reflections were collected, but only 708 were unique and not systematically absent. The reflections were corrected for Lorentz-polarization and secondary extinction effects (ref 3). No absorption correction was made. R for the averaging of intensities is 0.033.

From the observed systematic absences of reflections ($hkl: h+k=2n+1$), the space group was determined to be monoclinic C2 (no. 2).

A trial structure involving the non-hydrogen atoms was determined with direct methods (ref 4). All the hydrogen atoms were located with succeeding difference Fourier syntheses. Based on the trial structure, structure factors were calculated using the neutral atom scattering factors of Cromer and Waber (ref 5). Anomalous dispersion effects were also included in the calculations of the structure factors (ref 6) using Cromer's values for f' and f'' (ref 7).

Heavy atoms were refined anisotropically and hydrogen isotropically with full matrix least squares analysis. The final cycle of refinement based on 664 observed reflections

$$[I > 3\sigma(F_o)]$$

converged with an agreement factor (R) of 0.036 and a weighted agreement factor (R_w) of 0.044 where

$$R = (\sum |F_o| - |F_c|) / \sum |F_o|$$

and

$$R_w = \text{SQRT} [(\sum w |F_o| - |F_c|)^2 / \sum w |F_o|^2]$$

The maximum electron density peak on the final difference Fourier map was $0.21(6) \text{ e}/\text{\AA}^3$.

Pertinent crystallographic data, atomic coordinates, bond lengths and bond angles, torsion angles, and thermochemical data are presented in tables 1 to 5, respectively. The unit-cell packing is shown in figure 1, and the BDNPN molecule as well as its atom numbering scheme is depicted in figure 2. Newman diagrams which illustrate selected conformational details of the molecule are presented in figure 3.

RESULTS AND DISCUSSION

Crystal Structure

The reaction product crystallizes in the C-centered monoclinic space group C2 with unit-cell dimensions $a = 10.726(4) \text{ \AA}$, $b = 5.992(3) \text{ \AA}$, $c = 10.400(4) \text{ \AA}$, and $\beta = 110.01(3)^\circ$ (table 1).

The molecule lies on a crystallographic two-fold axis which passes through both its N(1)-N(2) bond and the unit-cell origin. The C2 space group symmetry operations generate two molecules per unit cell which results in a calculated density of 1.72 g/cc.

The molecular packing shown in figure 1 consists of molecules oriented parallel to the c axis at the unit-cell origin and 220. Each molecule has six nearest neighbors which are held together by molecular forces.

Molecular Structure of BDNPN

Figure 2 clearly shows that the reaction product molecule has a nitro group bonded to the central nitrogen atom (N2) which is also bonded to two propyl groups that are related to each other by 2-fold symmetry. In each propyl group there is a gem-dinitro group substituted on the beta carbon which is labeled C(2). This structure confirms that the reaction scheme produces the target molecule, BDNPN.

Some of the interatomic distances (table 3) in the molecular backbone appear to be shorter than normal or accepted single-bond length values (ref 8). For example, the C(1)-C(2) distance is $1.541(2) \text{ \AA}$ which is consistent with the C-C single bond-length [$1.541(3) \text{ \AA}$] but the C(2)-C(3) distance of $1.514(3) \text{ \AA}$ is significantly shorter. The C(1)-N(2) distance of $1.451(2) \text{ \AA}$ is also shorter than the normal C-N single bond-length for either 3 covalent nitrogen [$1.472(5) \text{ \AA}$] or 4 covalent nitrogen [$1.479(5) \text{ \AA}$].

The observed shortening of the C(3)-C(2) and C(1)-N(2) bonds may be due to inductive effects caused by the strongly electron withdrawing gem-dinitro group bonded to C(2).

It has been observed that the nitramine group can have either a planar conformation or a pyramidal conformation (ref 9). In the planar configuration, the N-N bond lies in the C-N-C plane (N-N bend angle is 0°), and the bonding hybridization is sp^2 . In these planar nitramines, N-N bond shortening has been observed. For this bonding configuration, the N-N bond shortening has been attributed to double bond conjugation of the unshared p-type electrons on the amino nitrogen with nitro group electron system.

The appropriate torsion angles (table 4) to illustrate the relationship between the N-N bond and the C-N-C plane in BDNPN, C(1)-N(2)-C(1)a-N(1) and N(2)-C(1)-C(1)a-N(1)a,

have values of 180.0 deg and 0.00 deg, respectively. These values indicate that the N(1)-N(2) bend angle is 0 deg, and that the resulting bonding hybridization is sp^2 .

The N(1)-N(2) distance of 1.367(3) Å falls within the range of N-N bond lengths observed in both cyclic and acyclic nitramines (ref 9). Since this distance is significantly shorter than the 'normal' single-bond distance of 1.44(4) Å, but longer than the 'normal' double-bond distance of 1.24(1) Å, this N-N bond can be considered a partial double bond. That is to say, the N(1)-N(2) bond order is greater than 1 and less than 2.

In the pyramidal configuration, the N-N is bent out of the C-N-C plane. Since the N-N bond does not lie in the C-N-N plane, some degree of sp^3 bonding hybridization is involved. The larger the bend angle, the greater is the sp^3 contribution and the N-N will have more single bond character. Hence, the N-N distance should be greater in pyramidal nitramines than in planar nitramines.

This pyramidal conformation is evident in TNAZ where the N-N bond bend angle is 39.4 (ref 9). Despite this large bend angle, however, the observed N-N distance of 1.351 Å is significantly shorter than both the normal N-N single bond-length and the N-N distance found in the planar BDNPN. In this case, the cause for bond shortening has been ascribed to inductive effects of the strongly electron withdrawing gem-dinitro group in the strained four-membered ring rather than to double bond conjugation in the nitramine group.

Despite the planarity of the N(1)-N(2) bond in BDNPN, the oxygen atoms of nitramino nitro group are twisted -3.2 deg out of the C(1)-N(1)-C(1) plane (table 4). This relatively small twist, which is illustrated by Newman diagram 1 in figure 4, probably is caused by steric repulsive interactions between the nitramino O(1) and the O(2) of the closer nitro group [O(2)-N(3)-O(3)]. In contrast to the nitramino group, the nitro group which is depicted by Newman diagram 3 in figure 4, is twisted -79.8 deg around its single bond [C(2)-N(3)]. Since the sigma bonding present in single bonds permits free rotation and the pi bonding found in double bonds restricts free rotation, it is reasonable to expect the single-bonded nitro group to twist more readily than the nitramino group with its partial double bond character. The effect of this twisting results in a dihedral angle between the close nitro plane and the nitramino plane of 34.5 deg and a separation of 3.643 Å between O(1) and O(2).

The more remote nitro group, O(5)-N(4)-O(4), is not twisted around its single bond [C(2)-N(4)]. In this case its greater distance from the nitramine [O(1)...O(4), 4.693(3) Å] precludes repulsive interactions between the two groups.

The N(3)-C(2)-N(4) bond angle is 102.4(1) deg, but because of the observed twist in one of the nitro groups, the angle between the planes of the gem-dinitro group is 79 deg (table 4).

Some pertinent thermochemical parameters of RDX, TNAZ, and DNPB presented in

table 5 were calculated with the MCVECE code (refs 10 and 11). A comparison of these data reveals that BDNPN has the lowest flame temperature and also the highest impetus and heat of explosion values within this group of energetic molecules. This suggests that BDNPN may have potential for use in future gun propellant formulations, or even as a possible substitute for RDX in current gun propellant formulations.

As a preliminary test to determine if BDNPN is a viable candidate to replace RDX, the thermochemistry of three similar formulations were modeled. Each formulation is identical in every respect except that each one contains a different oxidizer, but in the same weight percent. The three formulations are composed of 0.4% ethylcentralite, 7.6% BDNPF/A, 4% NC(12.6), 12% CAB, and 76% of RDX, TNAZ, and BDNPN, respectively. It must be noted that this formulation may not be the optimum formulation for all three oxidizers because of stoichiometric differences among them.

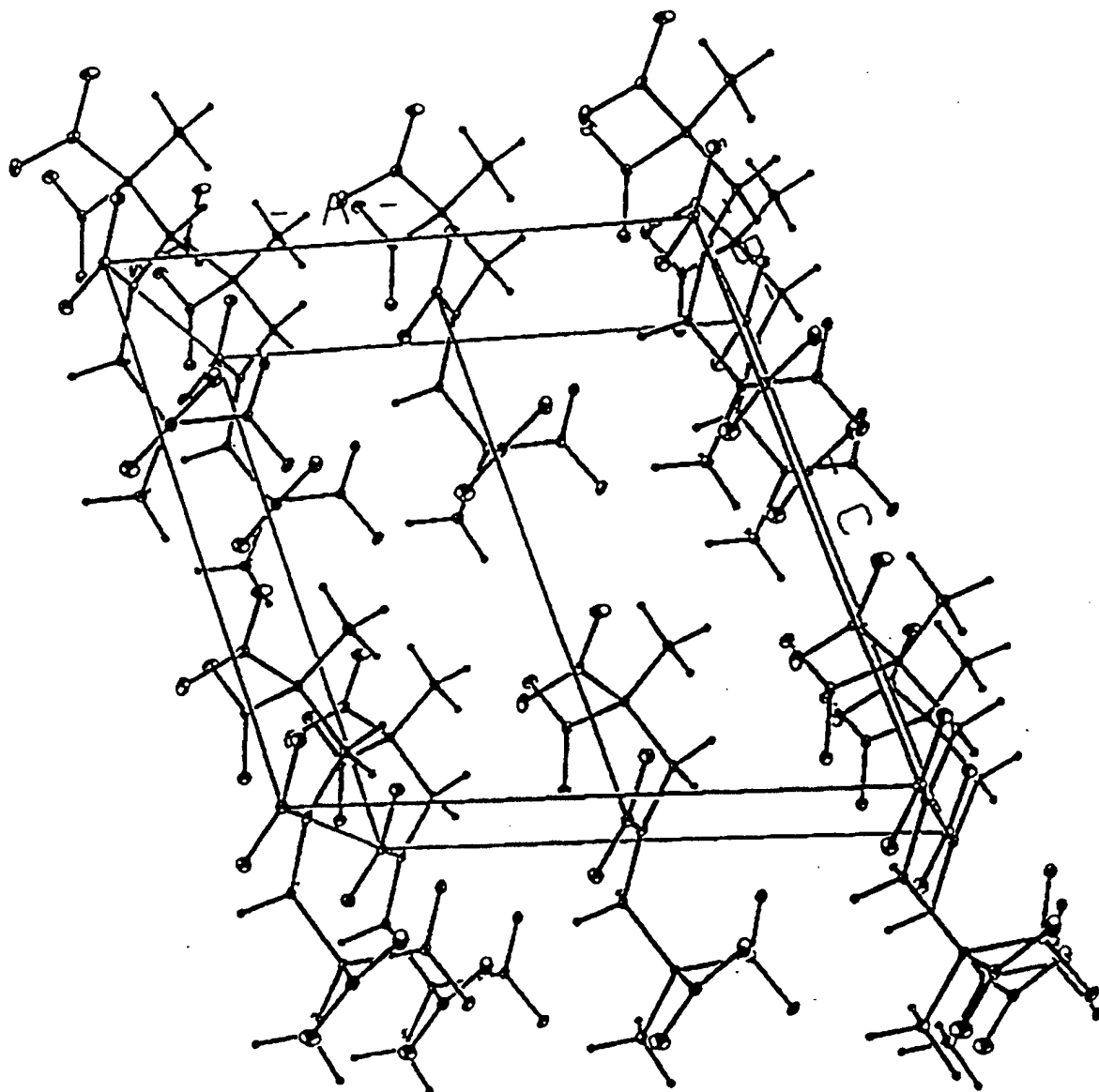
The modeling data (table 5) reveal that the BDNPN formulation yielded the lowest isochoric flame temperature (2948K) and an Impetus (1179 J/g) which is slightly less than that for the RDX formulation (1182 J/g) and slightly greater than that for the TNAZ formulation (1175 J/g).

CONCLUSIONS

1. BDNPN can be made from a relatively simple two-reaction process.
2. BDNPN is a planar nitramine-type molecule which also contains two gem-dinitro groups.
3. BDNPN is more energetic than either RDX or TNAZ, and it is also cooler burning.
4. The trial BDNPN propellant formulation is somewhat cooler burning than energetically comparable RDX and TNAZ formulations.
5. On an energetics basis, BDNPN should be considered a potential RDX replacement candidate.

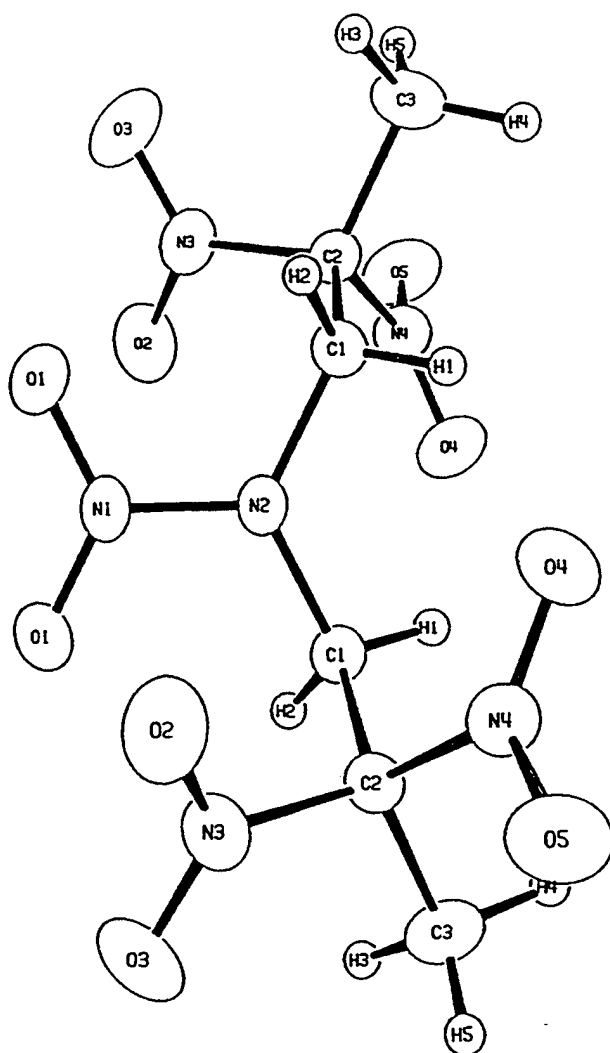
RECOMMENDATIONS

1. Synthesize sufficient quantity of BDNPN to characterize its chemical and physical properties.
2. Fabricate a small amount of an optimized BDNPN formulation and evaluate its properties.



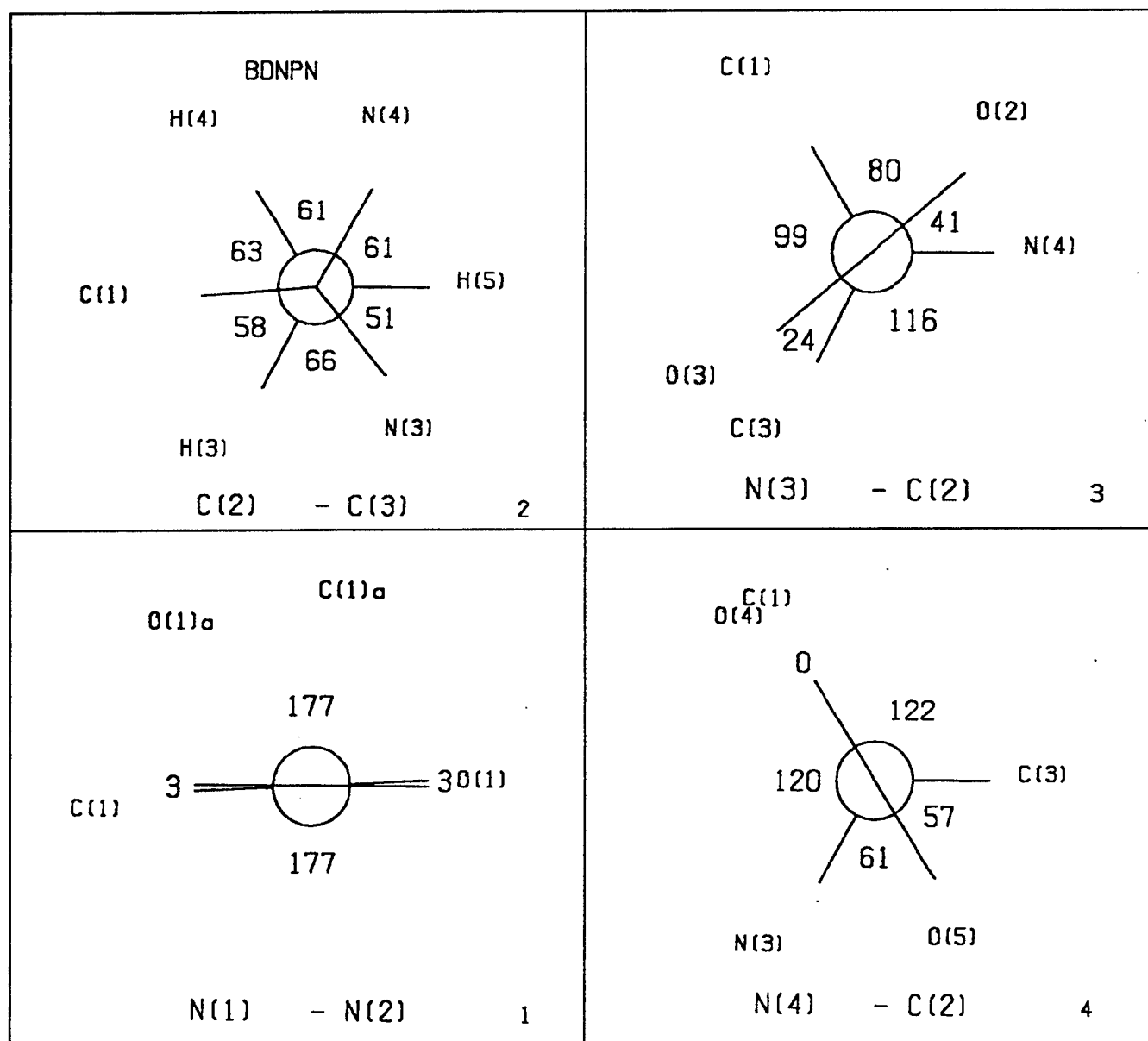
(Heavy-atom thermal ellipsoids are drawn at 40% probability while for better clarity the hydrogen atoms are represented by spheres of arbitrary size.)

Figure 1
Molecular packing of BDNPN viewed down the b axis of the unit cell



(Heavy-atoms are drawn at 40% probability while for better clarity the hydrogen atoms are represented by spheres of arbitrary size.)

Figure 2
BDNPN molecule and atom numbering scheme



1. N(1)-N(2)
2. C(2)-C(3)
3. N(3)-C(2)
4. N(4)-C(2)

Figure 3
Newman plots for bonds in BDNPN

Table 1
BDNPN crystallographic data¹

Molecule formula	C ₆ H ₁₀ N ₆ O ₁₂
Formula weight	326.8
Crystal system	monoclinic
Space group	C2 (no. 5)
a	10.726 (4) Å
b	5.992 (3) Å
c	10.400 (4) Å
β	110.01 (3) deg
V	628.1 Å ³
Z	2
D	1.72 g/cm ³
λ (Cu Kα)	1.541184 Å
u	14.8 cm ⁻¹
Scan type	w - 2θ
2θ max	150.0 deg
Total reflections	1345
Unique reflections	708
R	0.033
Extinction coef.	2.59E-05
R	0.036
Rw	0.044

¹ Data collected by Molecular Structure Corp., The Woodlands, TX.

Table 2
Atom coordinates and equivalent temperature factors with their ESDs in parentheses

<u>Atom</u>	<u>x/a</u>	<u>y/b</u>	<u>z/c</u>	<u>B_{eq}</u>
O(1)	0.0760(2)	-0.0934(3)	0.1011(2)	3.31(3)
O(2)	0.1119(2)	0.0688940	-0.2211(2)	4.45(4)
O(3)	-0.0784(2)	0.0397(4)	-0.3826(2)	5.40(5)
O(4)	0.1409(1)	0.5747(3)	-0.1029(1)	3.31(2)
O(5)	0.1288(1)	0.5253(4)	-0.3111(1)	4.38(4)
N(1)	0.0000	0.0000	0.0000	2.36(4)
N(2)	0.0000	0.2282(4)	0.0000	2.17(4)
N(3)	0.0020(2)	0.1375(4)	-0.2883(2)	3.03(3)
N(4)	0.0893(1)	0.4987(3)	-0.2155(2)	2.62(3)
C(1)	-0.0845(2)	0.3408(4)	-0.1222(2)	2.11(3)
C(2)	-0.0381(2)	0.3621(4)	-0.2464(2)	2.19(3)
C(3)	-0.1465(5)	0.4712(2)	-0.3634(2)	3.44(5)
H(1)	-0.097(2)	0.489(5)	-0.096(2)	2.2(4)
H(2)	-0.169(2)	0.276(5)	-0.159(2)	2.6(5)
H(3)	-0.230(2)	0.371(6)	-0.383(2)	3.7(6)
H(4)	-0.157(5)	0.629(7)	-0.327(3)	4.8(7)
H(5)	-0.125(3)	0.476(5)	-0.446(3)	4.0(6)

Table 3

Bond lengths in angstroms (Å) and bond angles in degrees with their ESDs in parentheses

<u>Atom</u>	<u>Atom</u>	<u>Distance</u>	<u>Atom</u>	<u>Atom</u>	<u>Atom</u>	<u>Angle</u>
C(1)	C(2)	1.542(2)	O(1)	N(1)	O(1)	125.6(3)
C(1)	N(2)	1.451(2)	O(1)	N(2)	N(2)	117.2(1)
C(1)	H(1)	0.95(3)	N(1)	N(2)	C(1)	117.7(1)
C(1)	H(2)	0.94(3)	C(1)	N(2)	C(1)	124.6(2)
C(2)	C(3)	1.514(3)	O(2)	N(3)	O(3)	125.6(2)
C(2)	N(3)	1.521(3)	O(2)	N(3)	C(2)	116.6(2)
C(2)	N(4)	1.530(2)	O(3)	N(3)	C(2)	117.8(2)
C(3)	H(3)	1.04(3)	O(4)	N(4)	O(5)	125.1(2)
C(3)	H(4)	1.04(4)	O(4)	N(4)	C(2)	119.2(1)
C(3)	H(5)	0.96(3)	O(5)	N(4)	C(2)	115.7(2)
N(1)	N(2)	1.367(3)	N(2)	C(1)	C(2)	119.2(1)
N(1)	O(1)	1.224(2)	N(2)	C(1)	H(1)	107.0(1)
N(3)	O(2)	1.218(3)	N(2)	C(1)	H(2)	113.0(2)
N(3)	O(3)	1.212(3)	C(2)	C(2)	H(1)	106.0(2)
N(4)	O(4)	1.201(2)	C(2)	C(1)	H(2)	104.0(1)
N(4)	O(5)	1.217(2)	H(1)	C(1)	H(2)	107.0(2)
			N(3)	C(2)	N(4)	102.4(1)
			N(3)	C(2)	C(1)	111.8(2)
			N(3)	C(2)	C(3)	111.5(2)
			N(4)	C(2)	C(1)	112.9(1)
			N(4)	C(2)	C(3)	108.9(2)
			C(1)	C(2)	C(3)	109.2(2)
			C(2)	C(3)	H(3)	106.0(2)
			C(2)	C(3)	H(4)	104.0(2)
			C(2)	C(3)	H(5)	112.0(2)
			H(3)	C(3)	H(4)	114.0(3)
			H(3)	C(3)	H(5)	107.0(2)
			H(4)	C(3)	H(5)	113.0(3)

Table 4
Selected torsion angles

<u>Atom 1</u>	<u>Atom 2</u>	<u>Atom 3</u>	<u>Atom 4</u>	<u>Angle</u>
C(1)	N(2)	C(1)a ²	N(1)	180.0
N(2)	C(1)	C(1)a	N(1)	0.0
O(2)	N(3)	C(2)	N(4)	41.4
O(2)	N(3)	C(2)	C(1)	- 79.7
O(2)	N(3)	C(c)	C(3)	157.7
O(3)	N(3)	C(2)	N(4)	- 140.4
O(3)	N(3)	C(2)	C(1)	98.4
O(3)	N(3)	C(2)	C(3)	- 24.3
O(4)	N(4)	C(2)	N(3)	- 120.3
O(4)	N(4)	C(2)	C(1)	0.1
O(4)	N(4)	C(2)	C(3)	121.6
O(5)	N(4)	C(2)	N(3)	61.3
O(5)	N(4)	C(2)	C(1)	- 178.3
O(5)	N(4)	C(2)	C(3)	- 56.8
N(2)	C(1)	C(2)	N(3)	52.3
N(2)	C(1)	C(2)	N(4)	- 62.5
N(2)	C(1)	C(2)	c(3)	176.2

² C(1)a is related to C(1) by 2-fold rotation axis.

Table 5
Thermochemical parameter (MCVEVCE) for oxidizers and their formulations

<u>Sample</u>	Impetus <u>J/g</u>	Flame temp <u>K</u>	Heat of expl <u>Cal/g</u>
Oxidizer			
RDX	1408	4101	1260
TNAZ	1403	4088	1278
BDNPN	1450	4016	1256
Formulation			
76% RDX	1181.9	3060.9	931
76% TNAZ	1175.5	3052.1	926
76% BDNPN	1179.1	2947.7	913

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